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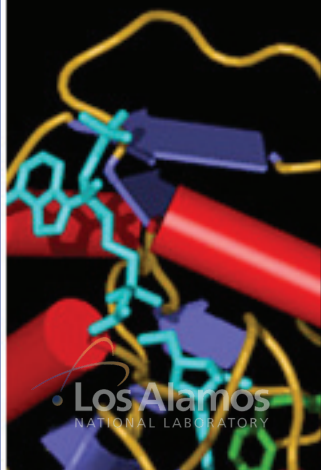
HEADS UP!

James Rhyne selected to be a Neutron Scattering Society of America Fellow



The Neutron Scattering Society of America selected James J. Rhyne to be a Fellow. He is cited "for extraordinary research on magnetic materials and thin films and outstanding leadership and support of major U.S. neutron facilities and research opportunities." Rhyne is the deputy group leader for science in the LANSCE-Lujan Center (LANSCE-LC). His primary research interests are magnetic exchange, anisotropy, and magnetostriction effects in rare earth metals and compounds with particular emphasis on rare earth metallic superlattices. Rhyne has authored more than 230 papers in physics and materials science, has written 12 book chapters and invited review chapters, and has presented more than 30 invited talks at national and international conferences. He is a Fellow of the American Physical Society and was awarded the *Doctor Honoris Causa* from the Université Henri Poincaré in Nancy, France. Rhyne joined the Laboratory in 2003.

The main goal of the Neutron Scattering Society of America (NSSA) is to stimulate, promote and broaden the use of neutron scattering in science, engineering and technology. Through the Fellows Program, the NSSA recognizes members who have made significant contributions to the neutron scattering community in North America in one or more of the following areas: advances in knowledge through original research and publication, innovative contributions in the application of neutron scattering, contributions to the promotion or development of neutron scattering techniques, and service and participation in the activities of the NSSA or neutron community. Each year, election to fellowship of the NSSA is limited to no more than one half of one percent of the membership. The new Fellows will be recognized at the 2010 American Conference on Neutron Scattering to be held in Ottawa, Canada in June.



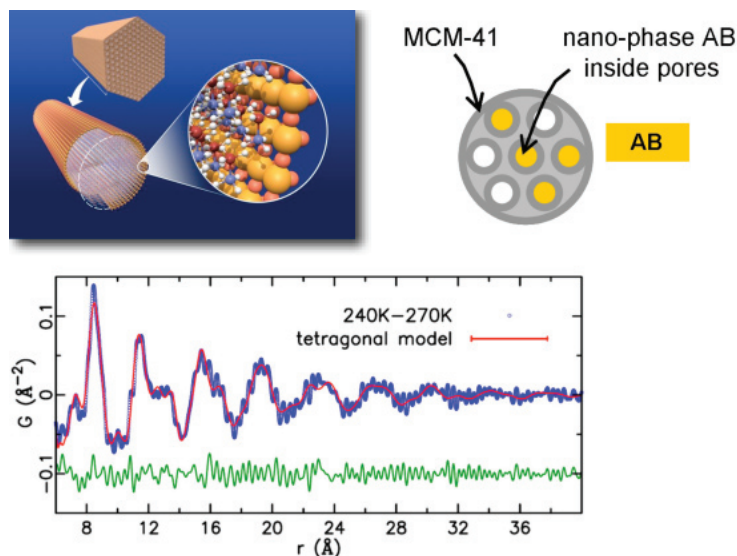
A nano look at ammonia borane and hydrogen storage

Molecular hydrogen is a potential clean energy source for fuel cells if the reactions to store and release hydrogen can be controlled. Scientists investigating ammonia borane (AB) as a high capacity hydrogen storage agent found that size reduction to the nanometer scale leads to enhanced hydrogen storage properties. When AB is packed into mesoporous silica, it releases higher quality hydrogen at more favorable temperatures than from its bulk form (see figure). Understanding the mechanism for this phenomenon is challenging because the light molecular ammonia borane (NH_3BH_3) nanocrystals must be identified inside the relatively heavy nano-containers of silica (SiO_2).

Hyunjeong Kim and Thomas Proffen (LANSC-E-LC) and collaborators from Pacific Northwest National Laboratory and Argonne National Laboratory examined how the nanosize packaging influences the structure and phase transition of AB. The team conducted synchrotron x-ray powder diffraction experiments on AB embedded within mesoporous silica, which contains approximately 4 nm-sized pores. The researchers collected data over the temperature range of 80K to 300K at Argonne National Laboratory's Advanced Photon Source. They used a local structural probing technique, called the atomic pair distribution function (PDF), to unravel the x-ray data (see figure).

The scientists found that AB molecules in silica are arranged in the same way as in the tetragonal phase of bulk form. However, nano-confined AB loses its well-ordered crystalline character and becomes amorphous above 270K. Such amorphization occurs at 343K in bulk form. Confined AB does not undergo the structural phase transition at 225K that the bulk form experiences. Instead, the molecular crystals retain their tetragonal phase over a temperature range from 110K to 270K. Therefore, less heat is needed to free the hydrogen when AB is confined in the mesoporous silica.

The results of the atomic pair distribution function analysis, combined with their earlier studies, suggest a possible means to control the hydrogen release reaction of hydrogen-rich molecules by the mesoporous silica packaging. The study also demonstrates how the atomic pair distribution function analysis could be applicable to investigate confined species, which cannot be analyzed by conventional structural probing techniques. A broad application of the technique to analyze encapsulated materials is possible. Reference: "Determination of Structure and Phase Transition of Light Element Nanocomposites in Mesoporous Silica: Case Study of NH_3BH_3 in MCM-4," *Journal of the American Chemical Society* **131** 13749 (2009). The Lujan Neutron Scattering Center, funded by the DOE Office of Basic Energy Sciences, supported the LANL research.



Schematic of the molecular configuration of the packed ammonia borane. AB is ammonia borane and MCM-41 is mesoporous silica. (Bottom): Changes in atomic pair distribution functions at 240K and 270K (blue open circle) are explained by the tetragonal structural model of bulk ammonia borane (red solid line). This indicates that ammonia borane inside MCM-41 has a tetragonal structure at 240K. The structural order is lost at 270 K, and it becomes amorphous. The green line is the difference between observed and measured pair distribution function.

Lujan Center studies structural materials for nuclear applications and highly irradiated steels

Peter Hosemann, Joris Van den Bosch and Stuart A. Maloy (MST-8); Amy Clarke (MST-6); Rex Hjelm (LANSC-E-LC); and collaborator G.R. Odette (University of California, Santa Barbara) conducted small angle neutron scattering (SANS) measurements on structural materials for nuclear applications. The purpose of this research was to measure particle density and particle size in oxide dispersion strengthened steels and carbide hardened materials, as well as radiation defect clusters and irradiation enhanced precipitation on samples irradiated at the Fast Flux Test Facility. SANS is used to characterize these types of structures at the National Institute of Standards and Technology, Paul Scherrer Institute in Switzerland, the GKSS Research Centre in Germany, and other research facilities. However, the low Q diffractometer at the Lujan Center is the only SANS instrument using time of flight, which allows scientists to gain additional data without moving the detector. Since the Lujan Center is a radiological controlled facility with well-organized radiological

continued on page 3

Structural... support, researchers are also able to investigate radioactive materials from reactor irradiations. The research using ferritic alloys requires the use of a high magnetic field (approximately 2T) to separate the neutron scattering signal from the magnetic scattering signal. This separation enables good contrast between the matrix material and the features of interest. Performing measurements on more than 50 samples at the Lujan Center has established SANS at LANL for this type of purpose. The figure shows a schematic of the experiment and SANS results on a friction stir welded oxide dispersion strengthened alloy (MA956). The reduction in the scattering signal on the welded material leads the scientists to the conclusion that no oxide particles remain after welding. The DOE Nuclear Energy - Fuel Cycle Research and Development Program (Stuart Maloy, LANL Program Manager) funded the work.

Technical contact: Peter Hosemann

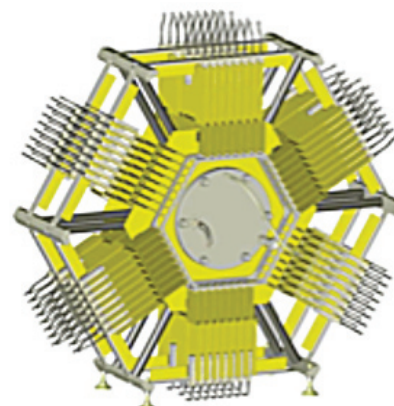
Nuclear Energy programs. Attendees included collaborators from LANSCE-NS, C-NR, Lawrence Livermore National Laboratory (LLNL), and Idaho National Laboratory (INL). Portions of these efforts are funded by Campaigns 1, 2 and 4 of the weapons program and by the Nuclear Data program of the Nuclear Energy office.

Fission cross sections and fission neutron output spectra are key quantities in modeling nuclear reactivity. As improvements are made in understanding materials properties and hydrodynamics of nuclear weapons, nuclear properties are a significant contributor to the overall uncertainty of predicted performance. The Chi Nu collaboration involving LANL, LLNL, INL, and university collaborators is developing techniques to measure fission neutron output spectra over the full incident and outgoing neutron energy ranges of interest. This work requires the new neutron detector arrays and associated digital data acquisition systems, which were a focus of this meeting.

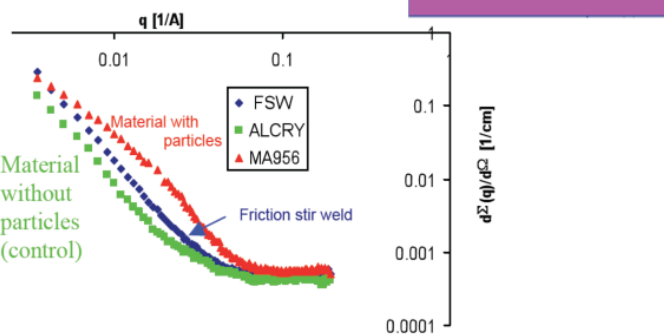
Technical contact: Robert Haight

A new approach to provide fission cross-sections with accuracies better than 1% uses a Time Projection Chamber that can track and identify all charged particles emitted from fission and from other reactions. This technique allows removal of backgrounds that limited the accuracy of previous measurements and enables a better understanding of systematic errors. The Time Projection Chamber was developed in collaboration between LANL, LLNL, INL, and six universities. The chamber was assembled at LLNL, and operation was tested using a radioactive source. The researchers will install the first prototype Time Projection Chamber at LANSCE in the upcoming accelerator beam cycle to start the commissioning phase. Tests of the time projection chamber in the LANSCE neutron beam are scheduled for the upcoming accelerator-running period. The participants evaluated and updated the multi-year project scope and progress at the meeting.

Technical contact: Fredrik Tovesson



Schematic of the Time Projection Chamber. The readout contains many thousands of channels of electronics that digitize the ionization tracks produced by charged particles of the gas in the chamber.



Schematic of the experiment at the LANSCE low Q diffractometer and resulting two-dimensional scattering pattern on the detector. (Bottom): Results on the oxide dispersion strengthened alloy MA956 as received, welded, and a control sample with no particles.

LANSCE-NS hosts national laboratories at fission measurements meeting

LANSCE-NS staff recently hosted a planning meeting on neutron-induced fission measurements. The meeting addressed ongoing collaborative projects to accurately measure the spectrum of neutrons emitted in fission and to attain an accuracy of less than 1% in the measured fission cross-sections. Both goals are priority items in the predictive capability framework of the Defense Programs Science Campaigns, and are important components of

Unraveling the mysteries of lipid domains in bio-membranes

Jaroslav Majewski and his student Mike Jablin (LANSCE-Lujan Center, LANSCE-LC) gave invited presentations describing their research on the structure and composition of lipid domains in cell biomembranes at the International Student Workshop on Lipid Domains, held at the Weizmann Institute of Science in Rehovot, Israel. The workshop's session "Biological membranes - are we on the same raft? A meeting of minds Between Chemistry, Physics and Biology," gathered chemists, physicists and biologists to discuss the challenge of understanding the structure and composition of lipid domains in the cell biomembranes.

Majewski's presentation, "Mixed Sphingomyelin/Cholesterol Layers and their Interactions with beta-Cyclodextrine: X-ray and Neutron Scattering Studies," examined the increasing evidence that lipids comprising the plasma membrane are inhomogeneously distributed, forming liquid domains rich in cholesterol and saturated lipids. These domains, also called lipid rafts, are implicated in many cell functions, such as endocytosis, signaling, and lipid regulation. Driving forces for lipid raft formation and the role cholesterol plays on membrane lipid organizations are unresolved. Beta-cyclodextrine can complex and remove cholesterol from membranes and also from cells in the human body.

Jablin elaborated in more detail on another of Majewski's research topics regarding "Thermoresponsive Polymer Supports Model Biomembranes," which examined novel model bio-membranes on polymeric cushions. The hybrid (bio/polymer) structure can better mimic the real cell's membranes than other model lipid membranes that reside on a solid, flat support. LANL's model lipid membrane is separated from the solid support by a polymeric cushion that can undulate, fluctuate, and change conformation like a real cell.

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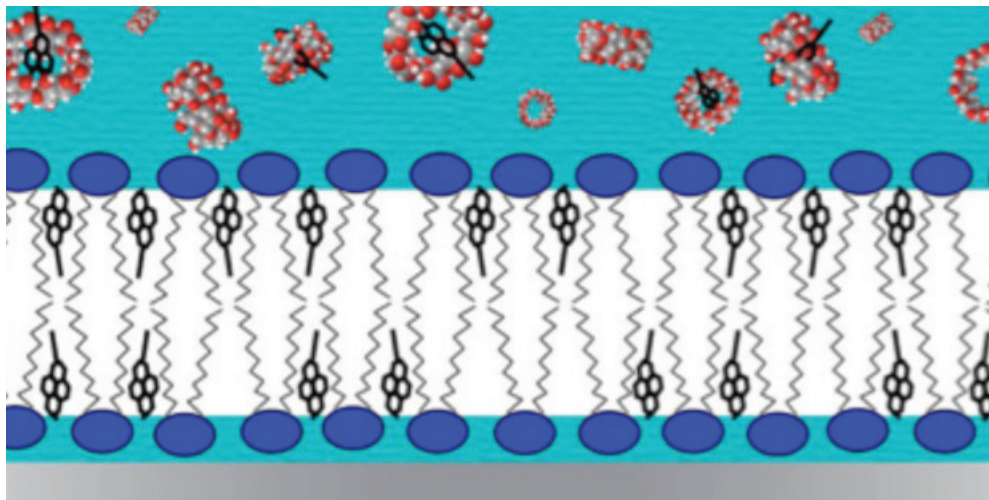
Celebrating Service

Congratulations to the following AOT and LANSCE employees celebrating service anniversaries this month:

Eric Pitcher, LANSCE-DO	30 years
Tsuyoshi Tajima, AOT-MDE	10 years
Patricia Herrera, LANSCE-DO	5 years

Majewski and Jablin collaborated with Manish Dubey (LANSCE-LC) and several scientists from Jagiellonian University in Poland (M. Flasiński, M. Broniatowski, and P. Dynarowicz-Latka). The DOE Office of Basic Energy Sciences funds the work.

Technical contact: Jaroslav Majewski



Schematic of beta-cyclodextrine (a component of some cholesterol lowering drugs) interacting with sphingomyelin/cholesterol domains. Red and white molecules depict beta-cyclodextrine. The black molecules represent cholesterol, and the blue molecules with black tails are sphingomyelin. The solid blue background is water.



2010

Accelerator and Electrodynamics Capability Review

May 17-20

HeadsUP!

WSST monthly hint

Working with chemicals in a research environment presents unique safety hazards. The nature of the work, with its unproven concepts, novel techniques, and unusual equipment demands that laboratory workers be alert to potential hazards. Never work in a vacuum—get independent help to review your proposed reactions!

For unknown reactions make sure you find a subject matter expert who can help identify hazards. Always start with small quantities of material and carefully observe reaction characteristics such as temperature, color, viscosity, and physical state. If possible, determine, from thermodynamic and kinetic considerations, the total quantity and the rate of evolution of heat and gases to be released during the reaction. Provide adequate cooling, ventilation, pressure relief, and gas purging. Isolate the reaction vessel, if possible, and make frequent inspections of equipment during reaction.

The chemical management ISD 101-14 available at int.lanl.gov/safety/chemical/docs/isd_tool3.pdf is a helpful tool for safely using chemicals.